Overview

Deriving scientific information from large, complex datasets can motivate large, complex statistical models; below we will give examples from our work on problems in astronomy, genomics, phylogenetics, econometrics, internet advertising, and ecology. As models grow in complexity, the need to interrogate their assumptions, to propagate uncertainty amongst their components, and to perform non-parametric checks on their data sensitivity grows commensurately. However, so does the computational cost of doing so using traditional statistical methods. Many classical procedures designed to address these concerns, such as Markov Chain Monte Carlo (MCMC), cross validation (CV), or re-estimating a model under a range of modeling assumptions, can be prohibitively expensive in many modern problems.

To help fill this gap, my research focuses on applications of *sensitivity analysis*, applied not merely in the traditional sense of assessing sensitivity to imprecise modeling assumptions (though I do pursue this traditional role as well), but also to assess freqeuntist sampling properties and propagate uncertainty in Bayesian procedures. At its core, my methodological work is all based on using Taylor series approximations, constructed only from properties of a single model fit, computed using either optimization or MCMC, to extrapolate to alternatives. In this way, I provide approximations to Bayesian posterior uncertainty, CV loss, and model sensitivity, while avoiding expensive re-estimation. Sensitivity analysis is a venerable idea with a rich existing literature, and I show that it has wide-ranging and fundamental applications in modern, computationally intensive statistical problems. Furthermore, I motivate the re-examination of theoretical ideas concerning the role of differential approximations in statistical analysis as practical tools in the age of big data and big computing.

I will divide my research statement into three parts: first, I will cover a more traditional application of sensitivity analysis to the assessment of prior sensitivity in Bayesian and variational Bayesian analysis. I will then discuss approximate CV and bootstrapping, which can be viewed as a kind of sensitivity analysis. Finally, I discuss how sensitivity analysis can recover accurate posterior covariances from variational Bayesian approximations, tying sensitiity analysis to the uniquitous scientific goal of uncertainty propagation.

Prior sensitivity in Bayesian analysis

Bayesian techniques allows analysts to reason coherently about unknown parameters, but only if the user specifies a complete generating process for the parameters and data, including both prior distributions for the parameters and precise likelihoods for the data. Often, aspects of this model are at best a considered simplifcation, and at worst chosen only for computational convenience. It is critical to ask whether the analysis would have changed substantively had different modeling choices been made.

Bayesian nonparametrics. A commonly question in unsupervised clustering is how many distinct clusters are present in a dataset. Discrete Bayesian nonparametrics (BNP) allows the answer to be inferred using Bayesian inference, but one must specify a prior on how distinct clusters are generated [Ghosh and Ramamoorthi, 2003, Gershman and Blei, 2012]. A particularly common modeling choice is the stick-breaking representation of a Dirichlet process prior [Sethuraman, 1994], a mathematical abstraction which is arguably better justified by its computational convenience than its realism. Our workshop paper, Giordano et al. [2018b], fits a BNP model with variational Bayes [Blei and Jordan, 2006] using the standard, computationally convenient stick-breaking prior, but then uses sensitivity analysis to allow the user to explore alternative functional forms an order of magnitude faster than would be possible with refitting. In work currently in progress, we apply our method to a human genome dataset in phylogenetics taken from [Huang et al., 2011], and find that our method accurately discovers real excess prior sensitivity in a BNP version of the model `fastSTRUCTURE` [Raj et al., 2014].

Partial pooling in meta-analysis. A popular form of meta-analysis in econometrics is to place a hierarchial model on a set of related experimental results, which both "shrinks" the individual estimates towards a common mean, potentially decreasing mean squared error, and allowing direct estimation of the average effect and diversity of effects [Rubin, 1981, Gelman and Rubin, 1992]. These advantages come at the cost of positing a precise generative process for the effects in question, and it is reasonable to interrogate whether the estimation procedure is robust to varaibility in these effects. In Giordano et al. [2016], we apply sensitivity analysis to a published meta-analysis of the effectiveness of microcredit interventions in seven developing countries [Meager, 2019]. We find that the conclusion are highly sensitive to the assumed covariance structure between the base level of business profitability and the microcredit effect, a covariance which is *a priori* difficult to ascertain, automatically diagnosing an important source of epistemic uncertainty not captured by the Bayesian posterior.

Hyperparameter sensitivity for MCMC. MCMC is arguably the most commonly used computational tool to estimate Bayesian posteriors, and modern black-box MCMC tools such as `Stan` [Stan Development Team, 2020, Carpenter et al., 2017]. However, MCMC still often takes a long time to run, and systematically exploring alternative prior parameterizations by re-running MCMC would be computationally prohibitive for all but the simplest models. A classical result from Bayesian robustness states that the sensitivity of a posterior expectation is given by a particular posterior covariance [Gustafson, 1996, Basu et al., 1996], though the result has not been widely used, arguably due in part to the lack of an automatic implementation. In my software package, Giordano [2020], I take advantage of the automatic differentiation capacities of `Stan` to provide automatic hyperparameter sensitivity for generic Stan models. In examples in the package `git` repository, I demonstrate the efficacy of the package in detecting

excess prior sensitivity, particularly in a social sciences model taken from Gelman and Hill [2006, Chapter 13.5].

Data sensitivity: cross validation and frequentist variance

Frequentist variability is ultimately concerned with the outcome of an estimation procedure if the data were drawn from the same distribution as but different from that observed. Similarly, all forms of cross-validation (CV) evaluates a statistic if parts of the observed data had been ablated. Both of these procedures can be treated by sensitivity analysis, where sensitivity is to the dataset itself.

Accuracy bounds for approximate cross validation. To perform leave-one-out CV (LOO-CV), one re-runs an estimation procedure with each datapoint left out. In full, LOO-CV requires as many re-runs procedures as there are datapoints, and each re-run is expected to be quite close to the original fit. Rather than re-running exactly, one can use a Taylor series to approximate the effect of removing a single data point; since the dataset with one point left out is, in some sense, "close" to the original dataset, the Taylor series can be expected to perform well.

Prior to our work, this idea had been suggested both in the machine learning literature [Rad and Maleki, 2018, Koh and Liang, 2017] as well as in the classical statistical literature under the name "infinitesimal jackknife" [Jaeckel, 1972, Shao and Tu, 2012]. However, the ML work appeared unaware of the statisical precedent, and both treatments required unrealistic theoretical conditions for the accuracy of the Taylor series: specifically, that the gradients of the objective function be uniformly bounded, a condition that is rarely satisfied in scientific practice, even in the simplest possible example of using maximum likelihood to estimate the sample mean of a normal distribution.

In Giordano et al. [2019b], we provide a more realistic set complexity condition under which the Taylor series is accurate, eschewing the need for bounded gradients, and synthesizing the classical statistics and ML literatures. Also unlike previous work, our theory was purely finite sample, implying the asymptotica results of prior work as a corollary. We demonstrated the accuracy of the technique on an unsupervised clustering problem from genomics [Shoemaker et al., 2015].

Sensitivity to removal of a small fraction of the data. Classical frequentist standard errors estimate the variability in an estimator that would result from the rarified thought experiment of re-sampling datsets from the same distribution that gave rise to the observed data. In the social sciences, this rarefied experiment rarely closely corresponds to reality, and one might be concerned if substantive conclusions could be overtuned by other minor perturbations to the data. For example, if a top-line conclusion of a study of the efficacy of cash transfers in a particular country [Angelucci and De Giorgi, 2009] could be reversed by removing a small percentage (say, 0.1%) of a dataset, one might

hesitate to generalize one's conclusions to other countries, even if the result was "statistically significant" according to classical frequentist standard errors.

In Giordano et al. [2020], we address this fundamental question, extending our earlier results in Giordano et al. [2019b]. We find that problems with small signal-to-noise ratio but large datasets will be particularly non-robust to the removal of a small proportion of the data. Such a situation that obtains commonly in econometrics, and we find that the sign and statistical significance of estimated effects in a number of large, prominent econometric studies can be overturned by dropping only a small number of datapoints [Angelucci and De Giorgi, 2009, Finkelstein et al., 2012]. Our robustness metric can be computed easily and automatically for any Z-estimator; we provide software and tractable finite-sample accuracy bounds for ordinary least squares and instrumental variables regression. More broadly, our work points to the importance of considering "practical significance" of effects in the social sciences rather than mere statistical significance.

Frequentist properties of Bayesian posteriors Bayesian measures is a powerful tool for coherently treating uncertainty in complex problems, but, when the model is misspecified, the estimated posterior uncertainty may not be meaningful. One can, however, always compute the frequentist sampling variability of a Bayesian posterior quantity, and such a quantity always remains meaningful, even if conceptually distinct from a posterior uncertainty Waddell et al. [2002], Kleijn and van der Vaart [2006], Huggins and Miller [2019].

By combining the frequentist IJ [Jaeckel, 1972, Shao and Tu, 2012, Giordano et al., 2019b] approach to frequentist variance with the MCMC-based measures of sensitivity [Gustafson, 2000, Giordano et al., 2018a], we are able to derive the Bayesian infinitesimal jackknife (IJ), which can be used to compute the frequentist variability of Bayeisan posterior means without bootstrapping or computing a maximum a-posteriori (MAP) estimate. In a work in progress, we extend the Bayesian central limit theorem of Lehmann and Casella [2006], Kass et al. [1990] to prove the consistency of the Bayesian IJ and show its accuracy as an approximation to the bootstrap for a larger number of examples, effectively allowing estimation of frequentist covariances orders of magnitude faster than the bootstrap. We demonstrate the accuracy of our method on datasets from election modeling [Gelman and Heidemanns, 2020], ecology [Kéry and Schaub, 2011], and most of the models from [Gelman and Hill, 2006, Stan Team, 2017].

Propagation of uncertainty in scalable Bayesian inference

Complex scientific inference procedures, such as the creation of astronomical catalogues, often exhibit uncertainty in many aspects of the model. For instance, in order to infer whether a handful of pixels on a telescopic image is a dim star or a distant galaxy, one must know the distortion (aka the point spread function) of the telescope, the lightness of the sky background, the noise of the photoreceptors, and the identity of nearby celestial objects, all of which quantities must themselves be inferred with some uncertainty.

Bayesian procedures coherently propagate uncertainty between all such model quantities, but classical MCMC procedures do not scale well, and are far beyond computational reach for astronomical catalogues. Researchers often turn to optimization-based mean field Variational Bayes (MFVB) procedures as a scalable alterative to MCMC, but MFVB does not estimate posterior correlations, and is known to underestimate marginal posterior uncertainties. [1]

In CITE, I develop a method to recover accurate posterior uncertainties from MFVB approximations without needing to fit a more complex model, or indeed to re-fit the original model. The idea is to exploit a duality between posterior covariances the sensitivity of posterior means and use the sensitivity of the MFVB approximation to infinitesimal perturbations as an estimator of the posterior covariance. We call the method "linear response variational Bayes" (LRVB) after the idea's progenitor as a method in statistical mechanics for inferring microscopic intensive thermodynamic quantities from macroscopic perturbations of extensive quantities. Computing the LRVB covaraince requires solving a linear system, which in scientific applications is often sparse and can be solved using iterative techniques such as conjugate gradient.

We compare LRVB covariances to MCMC on a large number of real-world datasets, including logistic regression on internet-scale data, the Cormack-Jolly-Seber model from ecology, and hierarchical generalized linear models from the social sciences, and demonstrated accurate posterior covariances computed over an order of magnitude faster than MCMC.

Selected Future work

There is a lot to be done simply applying the above methodology to applied problems in conjuction with collaborators with domain expertise. However, in this section, I will focus instead on new methodological directions suggested by the above work.

The bootstrap and the bootstrap after the bootstrap. Our work on the higher-order infinitesimal jackknife could be applied to other random reweighting schemes, particularly the bootstrap. The bootstrap is known to have frequentist properties that are asymptotically more accurate than the normal approximation in certain circumstances CITE, but the bootstrap requires re-computing an estimator as many time as there are bootstrap samples. However, a sufficiently high-order IJ estimate will approach the bootstrap estimator at a rate faster than the bootstrap's extra accuracy, strongly suggesting that the IJ will inherit all of the bootstrap's attractive properties at a fraction of the computational cost. The IJ is particularly appealing for bootstrap-after-bootstrap procedures, which have attractive theoretical properties but are computationally prohibitive even on medium-sized statistical problems. It seems plausible that the HOIJ could open up a range of bootstrap applications that are presently out of reach.

[1] The frequentist expectation-maximization, or EM, algorithm, can be understood as a MFVB procedure, and the present criticism applies to it as well.

Bayesian model criticism. Essentially all tools for checking the accuracy of Bayesian models are frequentist in nature — e.g. checking whether the data is likely under draws from the prior or posterior, or evaluating its predicive performance on a held-out dataset. Predictive model checks, such as leave-one-out CV are attractive, but currently have few practical implementations that avoid multiple runs of the MCMC algorithm. However, the possibility of forming higher-order expansions of the Bayesian posterior as a function of the empirical distribtuion could change that.

Partitioned Bayesian inference with theoretical bounds. Given a large, complicated problem, it is often computationally convenient to perform inference in separate computatoinal steps, while still propagating uncertainty from one step to another. For example, in CITE, we first fit spline regressions to time series of gene expression data, and then clustered the spline fits to group together genes with similar behavior. The Bayesian ideal, which is the simultaneous estimation of the clusters and spline regression, was too computationally prohibitive, and would intuitively have given a similar result to the sequential analysis, to the extent that the cluster center priors did not shrink the spline regressions too much.

Incorporating LRVB corrections into MFVB approximations.

Bootstrapping simulation-based inference. Giordano et al. [2019a] Efron and Tibshirani [1994] Hall [2013]

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